Matrix Product States: defeating the curse of dimensionality

F. Alexander Wolf

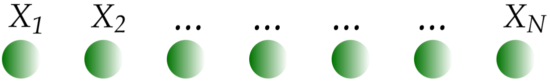
Arnold Sommerfeld Center for Theoretical Physics, LMU Munich

Columbia University, 23 Apr 2015

Outline

- ▷ MPS / Tensor Trains in statistical physics
- ▷ MPS in quantum mechanics

Generic example (i): noninteracting 1d Ising model

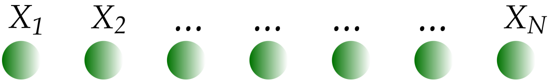


System described by vector of random variables $\boldsymbol{X} \in \{0,1\}^L$ with joint probability mass function

$$p(\boldsymbol{x}) = \tfrac{1}{Z} e^{-H(\boldsymbol{x})/T}, \quad H(\boldsymbol{x}) = \sum_{n=1}^{L} x_n$$

normalized with $Z = \sum_{\boldsymbol{x}} e^{-H(\boldsymbol{x})/T}$.

Generic example (i): noninteracting 1d Ising model



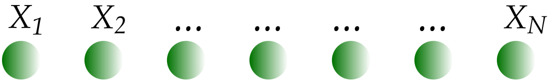
System described by vector of random variables $\boldsymbol{X} \in \{0,1\}^L$ with joint probability mass function

$$\boldsymbol{p}_{\boldsymbol{x}} = \tfrac{1}{Z} e^{-H(\boldsymbol{x})/T}, \quad H(\boldsymbol{x}) = \sum_{n=1}^{L} x_n$$

normalized with $Z = \sum_{\boldsymbol{x}} e^{-H(\boldsymbol{x})/T}$.

▷ $\boldsymbol{p}$ has 2^L components $\boldsymbol{x} \in \{(0,0,...,0),(0,0,...,1),\dots\}$.

Generic example (i): noninteracting 1d Ising model



System described by vector of random variables $\boldsymbol{X} \in \{0,1\}^L$ with joint probability mass function

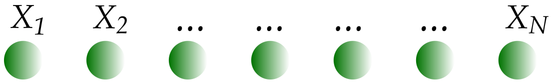
$$\boldsymbol{p}_{\boldsymbol{x}} = \tfrac{1}{Z} e^{-H(\boldsymbol{x})/T}, \quad H(\boldsymbol{x}) = \sum_{n=1}^{L} x_n$$

normalized with $Z = \sum_{\boldsymbol{x}} e^{-H(\boldsymbol{x})/T}$.

▷ $\boldsymbol{p}$ has 2^L components $\boldsymbol{x} \in \{(0,0,...,0),(0,0,...,1),\dots\}$.

▷ Remark $2^{100} \simeq 10^{30} \simeq 10^{15}$ TB.

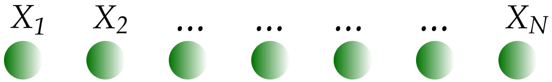
Generic example (i): noninteracting 1d Ising model



Compute correlations via $\mathrm{cov}(X_n, X_m) = \langle X_n X_m \rangle - \langle X_n \rangle \langle X_n \rangle$.

$$\langle X_n X_m \rangle = \sum_{\boldsymbol{x}} x_n x_m \boldsymbol{p}_{\boldsymbol{x}}$$

Generic example (i): noninteracting 1d Ising model



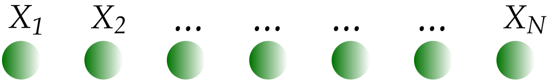
Compute correlations via $\text{cov}(X_n, X_m) = \langle X_n X_m \rangle - \langle X_n \rangle \langle X_n \rangle$.

$$\langle X_n X_m \rangle = \sum_{\boldsymbol{x}} x_n x_m \boldsymbol{p}_{\boldsymbol{x}}$$

▷ Naive brute force: 2^L operations necessary.

▷ Monte Carlo: sampling in space of 2^L states.

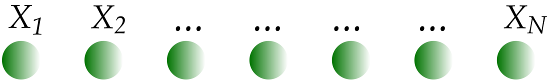
Generic example (i): noninteracting 1d Ising model



But: non-interacting degrees of freedom X_n imply full *separability*

$$
\begin{aligned}
\boldsymbol{p}_{\boldsymbol{x}} = \boldsymbol{p}_{x_1, x_2, \ldots, x_L} &= \frac{1}{Z} e^{-\sum_{n=1}^{L} x_n / T} \\
&= \frac{1}{Z} A_{x_1} A_{x_2} \ldots A_{x_L}, \quad A_{x_n} = e^{-x_n / T}
\end{aligned}
$$

Generic example (i): noninteracting 1d Ising model



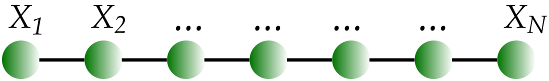
But: non-interacting degrees of freedom X_n imply full *separability*

$$\boldsymbol{p}_{\boldsymbol{x}} = \boldsymbol{p}_{x_1,x_2,\ldots,x_L} = \tfrac{1}{Z} e^{-\sum_{n=1}^{L} x_n/T}$$
$$= \tfrac{1}{Z} A_{x_1} A_{x_2} \ldots A_{x_L}, \quad A_{x_n} = e^{-x_n/T}$$

Compute correlations in $2L$ operations ...

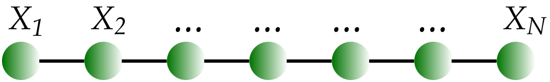
$$\langle X_n X_m \rangle = \frac{1}{Z} \Big(\sum_{x_n} x_n A_{x_n} \Big) \Big(\sum_{x_m} x_m A_{x_m} \Big) \prod_{k \neq n,m}^{L} \Big(\sum_{x_k} A_{x_k} \Big)$$
$$= \langle X_n \rangle \langle X_m \rangle \quad \ldots \quad \text{there are none.}$$

Generic example (ii): interacting 1d Ising model



$$\widetilde{\boldsymbol{p}}_{\boldsymbol{x}} = \tfrac{1}{Z} e^{-H(\boldsymbol{x})/T}, \quad H(\boldsymbol{x}) = -\sum_{n=1}^{L-1} x_n x_{n+1}$$

Generic example (ii): interacting 1d Ising model



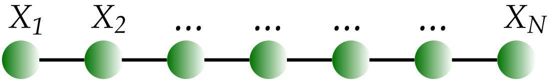
$$\widetilde{\boldsymbol{p}}_{\boldsymbol{x}} = \tfrac{1}{Z} e^{-H(\boldsymbol{x})/T}, \quad H(\boldsymbol{x}) = -\sum_{n=1}^{L-1} x_n x_{n+1}$$

▷ Is just a "discrete Gaussian" (continuous if $X_n \in \mathbb{R}$) with

$$\mathrm{cov}(\boldsymbol{x}, \boldsymbol{y})^{-1} = \begin{pmatrix} 0 & \frac{2}{T} & 0 & \dots & 0 \\ \frac{2}{T} & 0 & \frac{2}{T} & \dots & 0 \\ 0 & \frac{2}{T} & 0 & \frac{2}{T} & \dots \\ 0 & \ddots & \ddots & \ddots & \ddots \end{pmatrix}$$

▷ Correlations by inverting or diagonalizing the covariance matrix.

Generic example (ii): interacting 1d Ising model

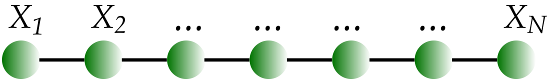


But: two-body interactions imply "almost – separability"

$$Z \sum_{\boldsymbol{x}} \widetilde{\boldsymbol{p}}_{\boldsymbol{x}} = \sum_{\boldsymbol{x}} e^{x_1 x_2 / T} e^{x_2 x_3 / T} \ldots$$

where gsum is the grand sum.

Generic example (ii): interacting 1d Ising model

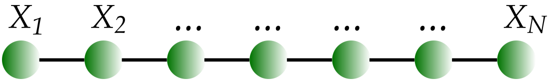


But: two-body interactions imply "almost – separability"

$$Z \sum_{\boldsymbol{x}} \widetilde{\boldsymbol{p}}_{\boldsymbol{x}} = \sum_{\boldsymbol{x}} A_{x_1,x_2} A_{x_2,x_3} \dots$$

where gsum is the grand sum.

Generic example (ii): interacting 1d Ising model



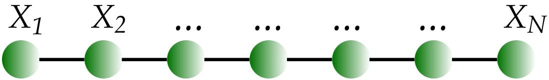
But: two-body interactions imply "almost – separability"

$$Z \sum_{\boldsymbol{x}} \widetilde{\boldsymbol{p}}_{\boldsymbol{x}} = \sum_{\boldsymbol{x}} A_{x_1,x_2} A_{x_2,x_3} \dots$$

$$= \mathsf{gsum} A A \dots, \qquad A_{x_n,x_{n+1}} = e^{x_n x_{n+1}/T}, \quad A \in \mathbb{R}^{2\times 2}$$

where gsum is the grand sum.

Generic example (ii): interacting 1d Ising model



But: two-body interactions imply "almost – separability"

$$Z\sum_{\boldsymbol{x}} \widetilde{\boldsymbol{p}}_{\boldsymbol{x}} = \sum_{\boldsymbol{x}} A_{x_1,x_2}A_{x_2,x_3}\dots$$

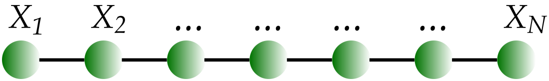
$$= \text{gsum} AA\dots, \qquad A_{x_n,x_{n+1}} = e^{x_n x_{n+1}/T}, \quad A\in\mathbb{R}^{2\times 2}$$

where gsum is the grand sum.

▷ Compare to non-interacting case

$$Z\sum_{\boldsymbol{x}} \boldsymbol{p}_{\boldsymbol{x}} = \sum_{\boldsymbol{x}} A_{x_1}A_{x_2}\dots, \qquad A_{x_n} = e^{-x_n/T}$$

Generic example (ii): interacting 1d Ising model

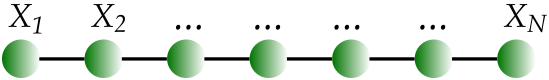


Compute correlations in $2^3 L$ operations (L matrix products)

$$\langle X_n X_m \rangle_{\widetilde{\boldsymbol{p}}} = \frac{1}{Z} \mathsf{gsum} \prod_{k=1}^{n-1} \left(A^{[k]} \right) M \prod_{k=n}^{m-1} \left(A^{[k]} \right) M \prod_{k=m}^{L-1} \left(A^{[k]} \right)$$

where $\quad M = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Generic example (ii): interacting 1d Ising model



Compute correlations in 2^3L operations (L matrix products)

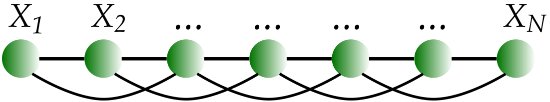
$$\langle X_n X_m \rangle_{\widetilde{\boldsymbol{p}}} = \frac{1}{Z} \mathsf{gsum} \prod_{k=1}^{n-1} \left(A^{[k]} \right) M \prod_{k=n}^{m-1} \left(A^{[k]} \right) M \prod_{k=m}^{L-1} \left(A^{[k]} \right)$$

where $M = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

▷ Compare to non-interacting case ($2L$ operations)

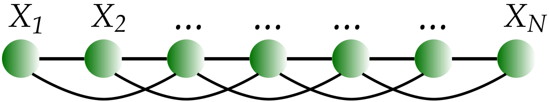
$$\langle X_n X_m \rangle_{\boldsymbol{p}} = \frac{1}{Z} \Big(\sum_{x_n} x_n A_{x_n} \Big) \Big(\sum_{x_m} x_m A_{x_m} \Big) \prod_{k \neq n,m} \Big(\sum_{x_k} A_{x_k} \Big)$$

Generic example (iii): three-body interacting Ising model



$$\hat{\boldsymbol{p}}_{\boldsymbol{x}} = \frac{1}{Z} e^{-H(\boldsymbol{x})/T}, \quad H(\boldsymbol{x}) = -\sum_{n=1}^{L-2} x_n x_{n+1} x_{n+2}$$

Generic example (iii): three-body interacting Ising model



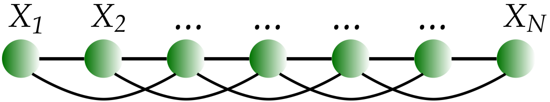
$$\hat{\boldsymbol{p}}_{\boldsymbol{x}} = \tfrac{1}{Z} e^{-H(\boldsymbol{x})/T}, \quad H(\boldsymbol{x}) = -\sum_{n=1}^{L-2} x_n x_{n+1} x_{n+2}$$

$$Z \sum_{\boldsymbol{x}} \hat{\boldsymbol{p}}_{\boldsymbol{x}} = \sum_{\boldsymbol{x}} \prod_{n=1}^{L-2} A_{x_n, x_{n+1}, x_{n+2}}$$

$$A_{x_n, x_{n+1}, x_{n+2}} = e^{x_n x_{n+1} x_{n+2}/T}$$

$$A \in \mathbb{R}^{2\times 2\times 2}$$

Generic example (iii): three-body interacting Ising model



$$\hat{\boldsymbol{p}}_{\boldsymbol{x}} = \frac{1}{Z} e^{-H(\boldsymbol{x})/T}, \quad H(\boldsymbol{x}) = -\sum_{n=1}^{L-2} x_n x_{n+1} x_{n+2}$$

$$Z \sum_{\boldsymbol{x}} \hat{\boldsymbol{p}}_{\boldsymbol{x}} = \sum_{\boldsymbol{x}} \prod_{n=1}^{L-2} A_{x_n, x_{n+1}, x_{n+2}}$$

$$A_{x_n, x_{n+1}, x_{n+2}} = e^{x_n x_{n+1} x_{n+2}/T}$$

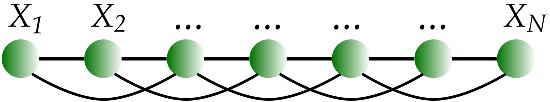
$$A \in \mathbb{R}^{2\times 2\times 2}$$

$$= \sum_{\boldsymbol{x}'} \prod_{n=1}^{L-2} B_{x'_n, x'_{n+1}} B^t_{x'_{n+1}, x'_{n+2}}$$

$$B_{x'_n, 2x_{n+1}+x_{n+2}} = A_{x_n, x_{n+1}, x_{n+2}}$$

$$B \in \mathbb{R}^{2\times 4}$$

Generic example (iii): three-body interacting Ising model



$$\hat{\boldsymbol{p}}_{\boldsymbol{x}} = \frac{1}{Z} e^{-H(\boldsymbol{x})/T}, \quad H(\boldsymbol{x}) = -\sum_{n=1}^{L-2} x_n x_{n+1} x_{n+2}$$

$$Z \sum_{\boldsymbol{x}} \hat{\boldsymbol{p}}_{\boldsymbol{x}} = \sum_{\boldsymbol{x}} \prod_{n=1}^{L-2} A_{x_n, x_{n+1}, x_{n+2}} \qquad A_{x_n, x_{n+1}, x_{n+2}} = e^{x_n x_{n+1} x_{n+2}/T}, \quad A \in \mathbb{R}^{2\times 2\times 2}$$

$$= \sum_{\boldsymbol{x}'} \prod_{n=1}^{L-2} B_{x'_n, x'_{n+1}} B^t_{x'_{n+1}, x'_{n+2}} \qquad B_{x'_n, 2x_{n+1}+x_{n+2}} = A_{x_n, x_{n+1}, x_{n+2}}, \quad B \in \mathbb{R}^{2\times 4}$$

Tensor Train format $\triangleright$ $\frac{1}{2}(2^3 + 4^3)L$ operations

Summary Part I

- Write probability mass function

$$p : \{0, 1, ..., d\}^L \to \mathbb{F}, \quad d, L \in \mathbb{N}$$

as vector

$$\boldsymbol{p}_{\boldsymbol{x}} = p(\boldsymbol{x}), \qquad \boldsymbol{p} \in \mathbb{F}^{d^L}$$

that is indexed *and parametrized* by $\boldsymbol{x} \in \{0, 1, ..., d\}^L$.

Summary Part I

- Write probability mass function

$$p : \{0, 1, ..., d\}^L \to \mathbb{F}, \quad d, L \in \mathbb{N}$$

as vector

$$\boldsymbol{p}_{\boldsymbol{x}} = p(\boldsymbol{x}), \qquad \boldsymbol{p} \in \mathbb{F}^{d^L}$$

that is indexed *and parametrized* by $\boldsymbol{x} \in \{0, 1, ..., d\}^L$.

If $\boldsymbol{p}_{\boldsymbol{x}} = v(\boldsymbol{x})$ does *not* couple *all* index components x_n among each other, there is a low rank MPS/TT representation.

Summary Part I

- Write probability mass function

$$p : \{0, 1, ..., d\}^L \to \mathbb{F}, \quad d, L \in \mathbb{N}$$

as vector

$$\boldsymbol{p}_{\boldsymbol{x}} = p(\boldsymbol{x}), \qquad \boldsymbol{p} \in \mathbb{F}^{d^L}$$

that is indexed *and parametrized* by $\boldsymbol{x} \in \{0, 1, ..., d\}^L$.

If $\boldsymbol{p}_{\boldsymbol{x}} = v(\boldsymbol{x})$ does *not* couple *all* index components x_n among each other, there is a low rank MPS/TT representation.

This reduces computational cost in summations over the $p(\boldsymbol{x})$ from exponential to linear in system size.

Summary Part I

- Write probability mass function

$$p : \{0, 1, ..., d\}^L \to \mathbb{F}, \quad d, L \in \mathbb{N}$$

as vector

$$\boldsymbol{p}_{\boldsymbol{x}} = p(\boldsymbol{x}), \qquad \boldsymbol{p} \in \mathbb{F}^{d^L}$$

that is indexed *and parametrized* by $\boldsymbol{x} \in \{0, 1, ..., d\}^L$.

If $\boldsymbol{p}_{\boldsymbol{x}} = v(\boldsymbol{x})$ does *not* couple *all* index components x_n among each other, there is a low rank MPS/TT representation.

This reduces computational cost in summations over the $p(\boldsymbol{x})$ from exponential to linear in system size.

- How to use this in quantum mechanics?

Outline

- MPS / Tensor Trains in statistical physics

- MPS in quantum mechanics

Statistical Mechanics – Quantum Mechanics

Instead of considering sums over classical weights, as in the partition sum,

$$1 = \sum_{\boldsymbol{x}} \boldsymbol{p}_{\boldsymbol{x}} = \sum_{\boldsymbol{x}} \langle \boldsymbol{x} | \hat{\boldsymbol{p}}_{\boldsymbol{x}} | \boldsymbol{x} \rangle,$$

where we used a somewhat exaggerated notation.

Statistical Mechanics – Quantum Mechanics

Instead of considering sums over classical weights, as in the partition sum,

$$1 = \sum_{\boldsymbol{x}} \boldsymbol{p_x} = \sum_{\boldsymbol{x}} \langle \boldsymbol{x} | \hat{\boldsymbol{p}}_{\boldsymbol{x}} | \boldsymbol{x} \rangle,$$

where we used a somewhat exaggerated notation. We now consider quantum many-body states

$$|\psi\rangle = \sum_{\boldsymbol{x}} \boldsymbol{c_x} | \boldsymbol{x} \rangle,$$

where $|\boldsymbol{x}\rangle = |x_1\rangle \otimes |x_2\rangle \otimes \cdots \otimes |x_L\rangle = |x_1 x_2 \ldots x_L\rangle$ is a tensor product of single-particle basis states $|x_i\rangle$. For example

$$|x_i\rangle \in \{| \uparrow_i\rangle, | \downarrow_i\rangle\}$$

Statistical Mechanics – Quantum Mechanics

Instead of considering sums over classical weights, as in the partition sum,

$$1 = \sum_{\boldsymbol{x}} \boldsymbol{p}_{\boldsymbol{x}} = \sum_{\boldsymbol{x}} \langle \boldsymbol{x} | \hat{\boldsymbol{p}}_{\boldsymbol{x}} | \boldsymbol{x} \rangle,$$

where we used a somewhat exaggerated notation. We now consider quantum many-body states

$$|\psi\rangle = \sum_{\boldsymbol{x}} \boldsymbol{c}_{\boldsymbol{x}} |\boldsymbol{x}\rangle,$$

where $|\boldsymbol{x}\rangle = |x_1\rangle \otimes |x_2\rangle \otimes \cdots \otimes |x_L\rangle = |x_1 x_2 \ldots x_L\rangle$ is a tensor product of single-particle basis states $|x_i\rangle$. For example

$$|x_i\rangle \in \{|\uparrow_i\rangle, |\downarrow_i\rangle\}$$

- But, do we know anything about how the vector of coefficients $\boldsymbol{c}_{\boldsymbol{x}}$ *couples* its components, so that the matrix product format is applicable?

For now we don't have to! Simply try the ansatz!

For now we don't have to! Simply try the ansatz!

- We can e.g. simply do a mean-field theory! Let us assume

$$\boldsymbol{c}_{\boldsymbol{x}} \overset{!}{=} a^{x_1} a^{x_2} \dots a^{x_L} = \prod_i a^{x_i}$$

then state can be manipulated doing $\sim L$ operations

$$|\psi\rangle = \sum_{\boldsymbol{x}} \boldsymbol{c}_{\boldsymbol{x}} |\boldsymbol{x}\rangle \overset{!}{=} |\psi_{\mathsf{MF}}\rangle = \sum_{\boldsymbol{x}} \prod_i a^{x_i} |\boldsymbol{x}\rangle = \prod_i^{\otimes} \Big(\sum_{x_i} a^{x_i} |x_i\rangle \Big)$$

For now we don't have to! Simply try the ansatz!

- We can e.g. simply do a mean-field theory! Let us assume

$$\boldsymbol{c_x} \overset{!}{=} a^{x_1} a^{x_2} \dots a^{x_L} = \prod_i a^{x_i}$$

then state can be manipulated doing $\sim L$ operations

$$|\psi\rangle = \sum_{\boldsymbol{x}} \boldsymbol{c_x} |\boldsymbol{x}\rangle \overset{!}{=} |\psi_{\mathsf{MF}}\rangle = \sum_{\boldsymbol{x}} \prod_i a^{x_i} |\boldsymbol{x}\rangle = \prod_i^{\otimes} \Big(\sum_{x_i} a^{x_i} |x_i\rangle \Big)$$

- How to determine the coefficients A^{x_i}? Variationally solve

$$\partial_{a^{x_i}} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = 0.$$

- Approximation to ground state. Approximation is *good* if ground state is in the same *class* of states as the ansatz $|\psi_{\mathsf{MF}}\rangle$.

What is a matrix product state? Schollwöck, arXiv:1008.3477 (2011)

- Relax mean-field assumption for coefficients of many body states

$$\boldsymbol{c_x} \overset{!}{=} a^{x_1} a^{x_2} a^{x_3} \ldots a^{x_L} = \prod_i a^{x_i}$$

to one that factorizes in matrices

$$\boldsymbol{c_x} \overset{!}{=} \sum_{\{\nu_i\}} A^{x_1}_{\nu_1} A^{x_2}_{\nu_1 \nu_2} A^{x_3}_{\nu_2 \nu_3} \ldots A^{x_L}_{\nu_L} = \prod_i A^{x_i}$$

What is a matrix product state? Schollwöck, arXiv:1008.3477 (2011)

- Relax mean-field assumption for coefficients of many body states

$$\boldsymbol{c_x} \stackrel{!}{=} a^{x_1} a^{x_2} a^{x_3} \dots a^{x_L} = \prod_i a^{x_i}$$

to one that factorizes in matrices

$$\boldsymbol{c_x} \stackrel{!}{=} \sum_{\{\nu_i\}} A^{x_1}_{\nu_1} A^{x_2}_{\nu_1 \nu_2} A^{x_3}_{\nu_2 \nu_3} \dots A^{x_L}_{\nu_L} = \prod_i A^{x_i}$$

- An MPS can be manipulated with costs of LD^3, where D is the dimension of the matrices A^{x_i}

$$|\psi\rangle = \sum_{\boldsymbol{x}} \boldsymbol{c_x} |\boldsymbol{x}\rangle \stackrel{!}{=} |\psi_{\text{MPS}}\rangle = \sum_{\boldsymbol{x}} \prod_i A^{x_i} |\boldsymbol{x}\rangle$$

What is a matrix product state? Schollwöck, arXiv:1008.3477 (2011)

- Relax mean-field assumption for coefficients of many body states

$$\boldsymbol{c_x} \stackrel{!}{=} a^{x_1} a^{x_2} a^{x_3} \dots a^{x_L} = \prod_i a^{x_i}$$

  to one that factorizes in matrices

$$\boldsymbol{c_x} \stackrel{!}{=} \sum_{\{\nu_i\}} A^{x_1}_{\nu_1} A^{x_2}_{\nu_1 \nu_2} A^{x_3}_{\nu_2 \nu_3} \dots A^{x_L}_{\nu_L} = \prod_i A^{x_i}$$

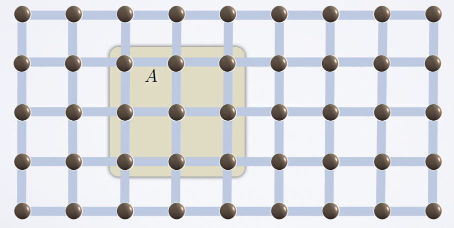
- An MPS can be manipulated with costs of LD^3, where D is the dimension of the matrices A^{x_i}

$$|\psi\rangle = \sum_{\boldsymbol{x}} \boldsymbol{c_x} |\boldsymbol{x}\rangle \stackrel{!}{=} |\psi_{\mathsf{MPS}}\rangle = \sum_{\boldsymbol{x}} \prod_i A^{x_i} |\boldsymbol{x}\rangle$$

- Are ground states in the same *class* as MPS? Which is this class? Are the coefficients $c_{\boldsymbol{x}}$ in ground states *weakly* coupled?

Class of lowly entangled states Eisert, arXiv:1308:3318 (2013)

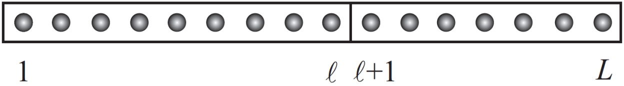
Many natural quantum lattice models have ground states that are little, in fact very little, entangled in a precise sense. This shows that "nature is lurking in some small corner of Hilbert space", one that can be essentially efficiently parametrized.



Gapped Hamiltonians with short range interactions.

- ▷ Physical correlations have a finite range.
- ▷ Entanglement fulfills **area law**: entanglement of a region A is proportional to surface $|\partial A|$, not volume $|A|$, of this region.

For a one-dimensional system? Schollwöck, arXiv:1008.3477 (2011)



$$|\psi\rangle = \sum_{\boldsymbol{x}_A} \sum_{\boldsymbol{x}_B} M_{\boldsymbol{x}_A \boldsymbol{x}_B} |\boldsymbol{x}_A\rangle |\boldsymbol{x}_B\rangle$$

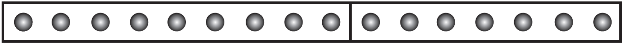
Perform SVD (singular value decomposition) $M = USV^\dagger$

- $U^\dagger U = I$ and $VV^\dagger = I$, i.e. U and V have columns of orthonormal vectors
- S is diagonal matrix

$$|\psi\rangle = \sum_{\nu} s_\nu |\nu\rangle_A |\nu\rangle_B$$

where $|\nu\rangle_A = \sum_{\boldsymbol{x}_A} U_{\boldsymbol{x}_A \nu} |\boldsymbol{x}_A\rangle$ and $|\nu\rangle_B = \sum_{\boldsymbol{x}_B} V^*_{\boldsymbol{x}_B \nu} |\boldsymbol{x}_B\rangle$

For a one-dimensional system? Schollwöck, arXiv:1008.3477 (2011)



Reduced density operators are readily obtained from

$$|\psi\rangle = \sum_{\nu} s_\nu |\nu\rangle_A |\nu\rangle_B$$

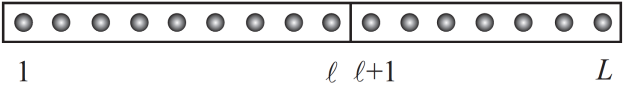
as trace over subsystem B can be performed easily

$$\rho_A = \mathrm{tr}_B |\psi\rangle\langle\psi| = \sum_{\nu} s_\nu^2 |\nu\rangle\langle\nu|$$

Entanglement between A and B

$$S_{A|B} = -\mathrm{tr}\rho_A \ln \rho_A = \sum_{\nu} s_\nu^2 \ln s_\nu^2$$

Relation with matrix product state? Schollwöck, arXiv:1008.3477 (2011)



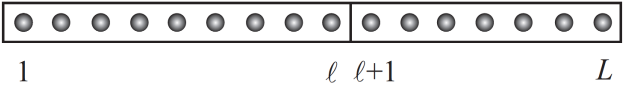
$$|\psi\rangle = \sum_{\nu} s_\nu |\nu\rangle_A |\nu\rangle_B$$

where $|\nu\rangle_A = \sum_{\boldsymbol{x}_A} U_{\boldsymbol{x}_A \nu} |\boldsymbol{x}_A\rangle$ and $|\nu\rangle_B = \sum_{\boldsymbol{x}_B} V^*_{\boldsymbol{x}_B \nu} |\boldsymbol{x}_B\rangle$

$$|\psi_{\text{MPS}}\rangle = \sum_{\boldsymbol{x}_A} \sum_{\boldsymbol{x}_B} \prod_{i=1}^{l} A^{x_i} \prod_{j=l+1}^{L} A^{x_j} |\boldsymbol{x}_A\rangle |\boldsymbol{x}_B\rangle$$

$$= \sum_{\nu} \underbrace{\sum_{\boldsymbol{x}_A} \left(\prod_{i=1}^{l} A^{x_i} \right)_{\nu} |\boldsymbol{x}_A\rangle}_{\sim |\nu\rangle_A} \underbrace{\sum_{\boldsymbol{x}_B} \left(\prod_{j=l+1}^{L} A^{x_j} \right)_{\nu} |\boldsymbol{x}_B\rangle}_{\sim |\nu\rangle_B,\ \text{up to unitary transform}}$$

Relation with matrix product state? Schollwöck, arXiv:1008.3477 (2011)



$$|\psi\rangle = \sum_{\nu} s_\nu |\nu\rangle_A |\nu\rangle_B$$

- As $\nu \in \{1, ..., D\}$, the matrix dimension D directly translates into number of allowed singular values, and by that the number of summands in the entanglement entropy!

$$S_{A|B} = -\mathrm{tr}\rho_A \ln \rho_A = \sum_{\nu} s_\nu^2 \ln s_\nu^2$$

- Mean-field states with matrix dimension 1 are not entangled!
- Everything up to D=1000 is easily treatable on a computer.

Summary

Sufficiently lowly entangled states can be efficiently represented by matrix product states. Fortunately, most physically relevant states are very lowly entangled.

- DMRG: Variational ground state search

$$\partial_{A^{\boldsymbol{x}_i}_{\mu\nu}} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = 0$$

  solved efficiently as ansatz is linear in $A^{\boldsymbol{x}_i}_{\mu\nu}$.
- Invention of DMRG: White, Phys. Rev. Lett. **69** 2863 (1992)
- Reviews: Schollwöck, Rev. Mod. Phys. **77**, 259 (2005) / Schollwöck, Annals of Physics **326**, 96 (2011)

Summary

Sufficiently lowly entangled states can be efficiently represented by matrix product states. Fortunately, most physically relevant states are very lowly entangled.

- DMRG: Variational ground state search

$$\partial_{A^{\boldsymbol{x}_i}_{\mu\nu}} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = 0$$

  solved efficiently as ansatz is linear in $A^{\boldsymbol{x}_i}_{\mu\nu}$.
- Invention of DMRG: White, Phys. Rev. Lett. **69** 2863 (1992)
- Reviews: Schollwöck, Rev. Mod. Phys. **77**, 259 (2005) / Schollwöck, Annals of Physics **326**, 96 (2011)

Thank you for your attention!

Schollwöck, U., 2005, Rev. Mod. Phys. **77**, 259.

Schollwöck, U., 2011, Annals of Physics **326**, 96.

White, S. R., 1992, Phys. Rev. Lett. **69**, 2863.